

Retraction of articles by H. Zhong *et al.*

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A series of 41 papers by H. Zhong *et al.* are retracted.

As a result of problems with the data sets and incorrect atom assignments, 41 papers by H. Zhong *et al.* are retracted. Full details of all the articles are given in Table 1.

**Table 1**

Details of articles to be retracted, in order of publication.

Title	Reference	DOI	Refcode
<i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thiourea solvate</i>	Zhong, Zeng, Liu & Luo (2006a)	10.1107/S1600536806041122	KERQEE
<i>cis-Dichlorobis(1,10-phenanthroline)cobalt(II)</i>	Zhong, Zeng & Luo (2006)	10.1107/S1600536806047295	MEQFOE
<i>Tris(quinolin-8-olato-κ<sup>2</sup>N,O)cobalt(III) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2006b)	10.1107/S1600536806050240	MEQHEW
<i>(8-Quinololinol-κ<sup>2</sup>N,O)bis(8-quinolinolato-κ<sup>2</sup>N,O)nickel(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Liu & Luo (2007)	10.1107/S1600536806053232	METVUD
<i>Aquachlorobis(1,10-phenanthroline)cobalt(II) chloride thioacetamide solvate</i>	Zhong, Zeng & Luo (2007)	10.1107/S1600536806053530	METQIM
<i>(8-Quinololinol-κ<sup>2</sup>N,O)-bis(8-quinolinolato-κ<sup>2</sup>N,O)zinc(II) glyoxal hemisolvate monohydrate</i>	Zhong, Zeng, Luo, Li & Xiao (2007)	10.1107/S1600536807001171	DEXTEG
<i>(Dimethylglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')nickel(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007a)	10.1107/S1600536807004102	YEYGOZ
<i>(Dimethylglyoxime-κ<sup>2</sup>N,N')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')zinc(II) dinitrate dihydrate</i>	Zhong, Zeng, Yang, Luo & Li (2007b)	10.1107/S1600536807004096	YEYGUF
<i>Chloridobis(1,10-phenanthroline-κN,N')copper(I) hexahydrate</i>	Zhong, Zeng, Yang, Luo & Xiao (2007)	10.1107/S160053680700791X	HEGKOU1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)cobalt(II)</i>	Zhong, Zeng, Yang & Luo (2007a)	10.1107/S1600536807017461	ITPCOO1
<i>Tetrakis(pyridine-κN)bis(thiocyanato-κN)copper(II)</i>	Zhong, Zeng, Yang & Luo (2007b)	10.1107/S160053680701879X	AVUJEG02
<i>Tetrakis(nitrato-κ<sup>2</sup>O,O')bis(4-phenylpyridine-κN)cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007c)	10.1107/S1600536807018831	CICDOI
<i>Bis(4,4'-bipyridine-κ<sup>2</sup>N,N')tetrakis(nitrato-κ<sup>2</sup>O,O')cerium(IV)</i>	Zhong, Zeng, Yang & Luo (2007d)	10.1107/S1600536807021502	YIDNEF
<i>(1,10-Phenanthroline)tris(phenoxyacetato)lanthanum(III)</i>	Zhong, Zeng, Yang, Luo & Xu (2007)	10.1107/S1600536807027171	EDUROL
<i>(1,10-Phenanthroline)tris(phenoxyacetato)cerium(III)</i>	Zhong, Yang, Luo & Xu (2007a)	10.1107/S1600536807028061	EDUTUT
<i>(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)</i>	Zhong, Yang, Luo & Xu (2007b)	10.1107/S1600536807028693	RIGQEE
<i>(1,10-Phenanthroline-κ<sup>2</sup>N,N')tris(phenoxyacetato)-κO;κO;κO,O'-neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007c)	10.1107/S1600536807030371	UDUMEM
<i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(thiocyanato-κN)nickel(II)</i>	Zhong, Yang, Luo & Xu (2007d)	10.1107/S1600536807031613	YEJGOJ01
<i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(isothiocyanato-κN)copper(II)</i>	Zhong, Yang, Luo & Xu (2007e)	10.1107/S1600536807033181	UFAPOH
<i>Bis(2,2'-bipyridyl-κ<sup>2</sup>N,N')bis(thiocyanato-κN)zinc(II)</i>	Zhong, Yang, Luo & Xu (2007f)	10.1107/S1600536807035337	TIGFAR
<i>(1,10-Phenanthroline-κ<sup>2</sup>N,N')tris(3-phenylpropanoato-κO)neodymium(III)</i>	Zhong, Yang, Luo & Xu (2007g)	10.1107/S1600536807035350	TIGFEV
<i>2-Fluoro-3,5-dinitrobenzamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007j)	10.1107/S1600536807038676	VIKGAY
<i>2-Fluoro-3,5-dinitrobenzoic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007k)	10.1107/S1600536807039724	KILKIA
<i>1-Hydroxy-4,6-dinitropyridine-2-carboxamide monohydrate</i>	Zhong, Yang, Xie & Luo (2007l)	10.1107/S1600536807040779	AFETAH
<i>N-(2-Hydroxyphenyl)carbamic acid-ammonia (1/1)</i>	Zhong, Yang, Xie & Luo (2007m)	10.1107/S160053680704086X	AFINAF
<i>catena-Poly[[bis(μ-anilinoacetato-κ<sup>2</sup>O:O')bis(μ-anilinoacetato-κ<sup>2</sup>O:O')bis(1,10-phenanthroline-κ<sup>2</sup>N,N')samarium(III)]-μ-anilinoacetato-κ<sup>2</sup>O:O']</i>	Zhong, Yang, Xie & Luo (2007a)	10.1107/S1600536807043528	PILDAQ
<i>2-Hydroxy-5-nitrobenzene-1,3-dicarboxylic acid monohydrate</i>	Zhong, Yang, Xie & Luo (2007n)	10.1107/S1600536807045199	XILWIZ
<i>catena-Poly[[tetra-μ-anilinoacetato-bis(1,10-phenanthroline)-dineodymium(III)]-di-μ-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007b)	10.1107/S1600536807048489	WIMWEV
<i>Hexaquaacopper(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007c)	10.1107/S1600536807049525	TOLSCV01

**Table 1 (continued)**

Title	Reference	DOI	Refcode
<i>catena-Poly[[tetra-<math>\mu</math>-anilinoacetato-bis(1,10-phenanthroline)-dilanthanum(III)]-di-<math>\mu</math>-anilinoacetato]</i>	Zhong, Yang, Xie & Luo (2007d)	10.1107/S1600536807051240	GIMZEI
<i>Hexaaquachromium(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007e)	10.1107/S1600536807051227	GIMZIM
<i>Hexaaquamanganese(II) bis(4-methylbenzenesulfonate)</i>	Zhong, Yang, Xie & Luo (2007f)	10.1107/S1600536807052051	QUKQES01
<i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')cobalt(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>	Zhong, Yang, Xie & Luo (2007g)	10.1107/S1600536807053494	NIQLAB
<i>Hexaaquanickel(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007a)	10.1107/S1600536807054372	HIPZOW
<i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')copper(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>	Zhong, Yang, Xie & Luo (2007h)	10.1107/S160053680705622X	XIRGOV
<i>Hexaaquazinc(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Zhong, Xie & Luo (2007b)	10.1107/S1600536807056498	XIRJEO
<i>catena-Poly[(acetato-<math>\kappa</math>O)(1,10-phenanthroline-<math>\kappa^2</math>N,N')nickel(II)]-<math>\mu</math>-acetato-<math>\kappa^2</math>O:O']</i>	Zhong, Yang, Xie & Luo (2007i)	10.1107/S1600536807058540	HIQJOH
<i>Hexaaquacobalt(II) bis(4-aminobenzenesulfonate)</i>	Zhong, Xie & Luo (2007)	10.1107/S1600536807058527	HIQJUN
<i>catena-Poly[[tetra-<math>\mu</math>-anilinoacetato-bis(1,10-phenanthroline)-dieuropium(III)]-di-<math>\mu</math>-anilinoacetato]</i>	Zhong, Yang, Duan & Hong (2007)	10.1107/S1600536807060643	YIQMAN
<i>(Dimethylglyoxime-<math>\kappa^2</math>N,N')bis(1,10-phenanthroline-<math>\kappa^2</math>N,N')copper(II) dinirate dihydrate</i>	Zhong, Yang, Luo & Li (2007)	10.1107/S1600536807061193	YIQNUI
<i>catena-Poly[(1,10-phenanthroline-<math>\kappa^2</math>N,N')praseodymium(III)]-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^4</math>O:O'-[(1,10-phenanthroline-<math>\kappa^2</math>N,N')praseodymium(III)]-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^4</math>O:O'-di-<math>\mu</math>-phenoxyacetato-<math>\kappa^3</math>O,O':<math>\kappa^3</math>O:O,O']</i>	Zhong, Yang, Luo & Xu (2008)	10.1107/S1600536807068614	GISJIC

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**(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)**H. Zhong,<sup>a\*</sup> X.-M. Yang,<sup>b</sup> Q.-Y. Luo<sup>a</sup> and Y.-P. Xu<sup>a</sup>

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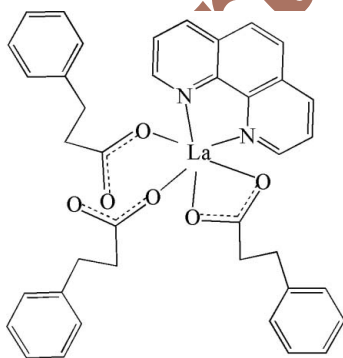
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Key indicators: single-crystal X-ray study;  $T = 273$  K; mean  $\sigma(\text{C}-\text{C}) = 0.014$  Å;  $R$  factor = 0.041;  $wR$  factor = 0.171; data-to-parameter ratio = 19.4.

The La<sup>III</sup> atom in the title complex,  $[\text{La}(\text{C}_9\text{H}_9\text{O}_2)_3(\text{C}_{12}\text{H}_8\text{N}_2)]$ , is coordinated by two N atoms of a 1,10-phenanthroline (phen) ligand and four O atoms of three phenylpropanoate ligands. This mononuclear complex is further extended into a supramolecular network structure *via* nonclassical hydrogen bonds between CH groups of 1,10-phenanthroline or phenylpropanoate and O atoms of neighbouring phenylpropanoate ligands.

**Related literature**

For related literature, see: Allen *et al.* (1987); Daiguebonne *et al.* (2000); Farrugia *et al.* (2000); Kay *et al.* (1972); Ma *et al.* (1999); Mao *et al.* (1998); Starynowicz (1991, 1993); Tsukube & Shinoda (2002); Zhang *et al.* (2005); Zeng *et al.* (2000).

**Experimental***Crystal data*

$[\text{La}(\text{C}_9\text{H}_9\text{O}_2)_3(\text{C}_{12}\text{H}_8\text{N}_2)]$   
 $M_r = 766.60$

Monoclinic,  $P2_1/n$   
 $a = 19.904$  (3) Å  
 $b = 8.783$  (5) Å  
 $c = 21.012$  (2) Å  
 $\beta = 106.163$  (2)°

$V = 3528$  (2) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 1.26$  mm<sup>-1</sup>  
 $T = 273$  (2) K  
 $0.33 \times 0.12 \times 0.08$  mm

*Data collection*

Bruker APEXII area-detector diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.682$ ,  $T_{\max} = 0.907$

26367 measured reflections  
7231 independent reflections  
4916 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.042$

*Refinement*

$R[F^2 > 2\sigma(F^2)] = 0.041$   
 $wR(F^2) = 0.171$   
 $S = 0.96$   
7231 reflections  
373 parameters

4 restraints  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 1.05$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.18$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1 $\cdots$ O2 <sup>i</sup>	0.93	2.44	3.138 (10)	132
C12—H12 $\cdots$ O5 <sup>ii</sup>	0.93	2.53	3.087 (9)	119
C32—H32B $\cdots$ O4 <sup>iii</sup>	0.97	2.48	3.435 (9)	167
C10—H10 $\cdots$ O7 <sup>iv</sup>	0.93	2.39	3.279 (9)	159

Symmetry codes: (i)  $-x+2, -y, -z+2$ ; (ii)  $-x+2, -y+1, -z+2$ ; (iii)  $x, y-1, z$ ; (iv)  $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$ .

Data collection: SMART (Siemens, 1996); cell refinement: SAINT (Siemens, 1996); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Siemens, 1996); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2323).

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**supplementary materials**

**Article retracted**

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## (1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)

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### Comment

In recent years, there has been great interest in the synthesis of metal organic frameworks (MOFs) with organic ligands and rare earth metals because of their novel structures, fascinating properties and important roles in special materials having optical, electronic, magnetic and biological importance potential applications (Deborah *et al.*, 2000; Farrugia *et al.*, 2000; Tsukube & Shinoda, 2002; Zhang *et al.*, 2005). These compounds are usually prepared by the reaction of rare-earth metal ions with bi- or multidentate ligands (Starynowicz, 1991, 1993; Kay *et al.*, 1972; Ma *et al.*, 1999; Zeng *et al.*, 2000; Mao *et al.*, 1998). We report herein the crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The six-coordinate environment of the La atom is completed by The two N atoms of 1,10-phenanthroline ligand and four O atoms of three benzenepropanoic acid ligands (Table 1). The La—O bond lengths are in the range 2.478 (4) to 2.908 (6) Å. The La—N bond lengths are in the range 2.717 (6) to 2.749 (5) Å. C—H...O non-classical hydrogen bonds between C—H groups of 1,10-phenanthroline or benzenepropanoic acid and O atoms of neighbouring benzenepropanoic acid molecules, with an average C...O distances of 3.235 (10) Å, generate a layered hydrogen-bonded network (Fig. 2 and Table 2). The non-classical hydrogen-bonding interactions link the mononuclear complex into a supramolecular network structure.

### Experimental

Crystals of the title compound were synthesized using hydrothermal method in a 23 ml Teflon-lined Parr bomb, which was then sealed. Lanthanum (III) chloride hexahydrate (106.1 mg, 0.3 mmol), phen (59.4 mg, 0.3 mmol), benzenepropanoic acid (90.1 mg, 0.6 mmol) and distilled water (3.5 g) were placed into the bomb and sealed. The bomb was then heated under autogenous pressure up to 423 K over the course of 7 d and allowed to cool at room temperature for 24 h. Upon opening the bomb, a clear colourless solution was decanted from small colourless crystals. These crystals were washed with distilled water followed by ethanol, and allowed to air-dry at room temperature.

### Refinement

H atoms were positioned geometrically, with C—H = 0.93 – 0.97 Å, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Figures

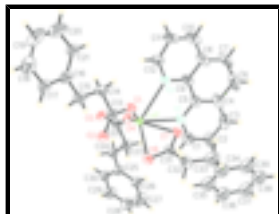


Fig. 1. View of the molecule of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

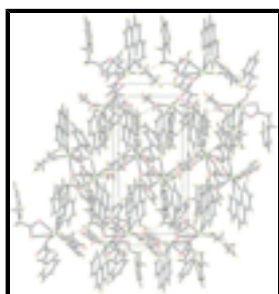


Fig. 2. A packing diagram of (I). Hydrogen bonding interactions are shown as dashed lines.

**(1,10-Phenanthroline)tri(3-phenylpropanoato)lanthanum(III)**

*Crystal data*

[La(C<sub>9</sub>H<sub>9</sub>O<sub>2</sub>)<sub>3</sub>(C<sub>12</sub>H<sub>8</sub>N<sub>2</sub>)]

$M_r = 766.60$

Monoclinic,  $P2_1/n$

Hall symbol: -P 2yn

$a = 19.904 (3) \text{ \AA}$

$b = 8.783 (5) \text{ \AA}$

$c = 21.012 (2) \text{ \AA}$

$\beta = 106.163 (2)^\circ$

$V = 3528 (2) \text{ \AA}^3$

$Z = 4$

$F_{000} = 1552$

$D_x = 1.443 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 9043 reflections

$\theta = 2.5\text{--}26.9^\circ$

$\mu = 1.26 \text{ mm}^{-1}$

$T = 273 (2) \text{ K}$

Plane, colourless

$0.33 \times 0.12 \times 0.08 \text{ mm}$

*Data collection*

Bruker APE XII area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 273(2) \text{ K}$

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.682$ ,  $T_{\max} = 0.907$

26367 measured reflections

7231 independent reflections

4916 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\max} = 26.6^\circ$

$\theta_{\min} = 2.0^\circ$

$h = -25 \rightarrow 24$

$k = -10 \rightarrow 11$

$l = -26 \rightarrow 26$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.171$	$w = 1/[\sigma^2(F_o^2) + (0.1521P)^2 + 0.285P]$
$S = 0.96$	where $P = (F_o^2 + 2F_c^2)/3$
7231 reflections	$(\Delta/\sigma)_{\max} = 0.003$
373 parameters	$\Delta\rho_{\max} = 1.05 \text{ e } \text{\AA}^{-3}$
4 restraints	$\Delta\rho_{\min} = -1.18 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
La1	0.931195 (16)	0.19073 (4)	0.964267 (15)	0.04126 (16)
O1	0.9710 (2)	0.0605 (5)	0.8751 (2)	0.0567 (11)
O2	1.0666 (2)	-0.0830 (6)	0.9217 (2)	0.0606 (12)
O4	0.9402 (2)	0.4212 (5)	1.0342 (2)	0.0565 (11)
O5	1.0078 (3)	0.6126 (6)	1.0912 (2)	0.0669 (13)
O7	0.8464 (2)	-0.0365 (5)	0.9192 (2)	0.0536 (10)
O8	0.9469 (2)	-0.1380 (6)	0.9773 (2)	0.0588 (11)
N1	0.7968 (3)	0.2345 (7)	0.9665 (3)	0.0577 (13)
N2	0.8346 (3)	0.3067 (6)	0.8549 (3)	0.0562 (14)
C1	0.7780 (4)	0.1909 (9)	1.0205 (4)	0.073 (2)
H1	0.8126	0.1683	1.0592	0.088*
C2	0.7095 (5)	0.1790 (11)	1.0201 (5)	0.096 (3)
H2	0.6974	0.1487	1.0578	0.115*
C3	0.6579 (5)	0.2135 (12)	0.9613 (6)	0.103 (4)
H3	0.6111	0.2053	0.9605	0.123*
C4	0.6744 (4)	0.2596 (13)	0.9041 (5)	0.088 (3)
C5	0.7461 (4)	0.2671 (8)	0.9093 (4)	0.0613 (17)

## supplementary materials

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C6	0.6192 (6)	0.2951 (16)	0.8423 (7)	0.137 (6)
H6	0.5720	0.2859	0.8398	0.165*
C7	0.6419 (5)	0.3449 (14)	0.7854 (5)	0.111 (4)
H7	0.6091	0.3711	0.7459	0.133*
C8	0.7127 (5)	0.3529 (11)	0.7907 (4)	0.083 (3)
C9	0.7658 (4)	0.3097 (7)	0.8501 (4)	0.0601 (19)
C10	0.7367 (6)	0.4012 (12)	0.7367 (4)	0.096 (3)
H10	0.7048	0.4318	0.6975	0.116*
C11	0.8049 (6)	0.4030 (11)	0.7419 (4)	0.092 (3)
H11	0.8210	0.4403	0.7074	0.110*
C12	0.8525 (5)	0.3479 (9)	0.8001 (4)	0.072 (2)
H12	0.8993	0.3395	0.8007	0.086*
C13	1.0282 (3)	0.0026 (7)	0.8772 (3)	0.0506 (14)
C14	1.0520 (3)	0.0495 (8)	0.8169 (3)	0.0573 (9)
H14A	1.0179	0.0163	0.7767	0.069*
H14B	1.0557	0.1595	0.8155	0.069*
C15	1.1171 (3)	-0.0166 (8)	0.8208 (3)	0.0573 (9)
H15A	1.1499	0.0168	0.8617	0.069*
H15B	1.1124	-0.1261	0.8236	0.069*
C16	1.1455 (3)	0.0142 (8)	0.7698 (3)	0.0573 (9)
C17	1.2069 (5)	-0.0559 (12)	0.7763 (5)	0.095 (3)
H17	1.2272	-0.1153	0.8133	0.113*
C18	1.2400 (5)	-0.0370 (14)	0.7251 (6)	0.108 (3)
H18	1.2821	-0.0858	0.7276	0.129*
C19	1.2087 (7)	0.0555 (13)	0.6709 (7)	0.119 (4)
H19	1.2310	0.0683	0.6377	0.142*
C20	1.1488 (7)	0.1251 (15)	0.6652 (6)	0.122 (4)
H20	1.1288	0.1844	0.6281	0.146*
C21	1.1144 (5)	0.1094 (12)	0.7162 (5)	0.096 (3)
H21	1.0729	0.1607	0.7139	0.115*
C22	0.9691 (3)	0.4986 (7)	1.0859 (3)	0.0522 (15)
C23	0.9485 (4)	0.4458 (8)	1.1470 (3)	0.0543 (9)
H23B	0.8987	0.4610	1.1397	0.065*
H23A	0.9580	0.3377	1.1535	0.065*
C24	0.9861 (4)	0.5271 (8)	1.2062 (3)	0.0543 (9)
H24A	1.0357	0.5149	1.2110	0.065*
H24B	0.9755	0.6345	1.1986	0.065*
C25	0.9745 (4)	0.4892 (7)	1.2653 (3)	0.0543 (9)
C26	0.9276 (4)	0.3793 (12)	1.2714 (4)	0.084 (2)
H26	0.9016	0.3257	1.2346	0.101*
C27	0.9198 (7)	0.3499 (16)	1.3343 (5)	0.126 (5)
H27	0.8900	0.2724	1.3397	0.151*
C28	0.9559 (6)	0.4345 (15)	1.3892 (5)	0.115 (4)
H28	0.9470	0.4187	1.4299	0.137*
C29	1.0048 (5)	0.5416 (13)	1.3838 (4)	0.102 (3)
H29	1.0305	0.5945	1.4210	0.122*
C30	1.0153 (4)	0.5697 (10)	1.3218 (4)	0.082 (2)
H30	1.0485	0.6403	1.3174	0.099*
C31	0.8838 (3)	-0.1527 (8)	0.9391 (3)	0.0517 (15)



C32	0.8576 (4)	-0.3131 (8)	0.9188 (4)	0.0626 (19)
H32A	0.8759	-0.3452	0.8827	0.075*
H32B	0.8769	-0.3808	0.9559	0.075*
C33	0.7861 (6)	-0.3313 (11)	0.8993 (6)	0.1096 (14)
H33A	0.7668	-0.2589	0.8641	0.132*
H33B	0.7760	-0.4324	0.8806	0.132*
C34	0.7529 (7)	-0.3143 (9)	0.9451 (7)	0.1096 (14)
C35	0.7848 (7)	-0.2738 (12)	1.0127 (7)	0.1096 (14)
H35	0.8325	-0.2547	1.0288	0.132*
C36	0.7374 (6)	-0.2645 (13)	1.0548 (7)	0.1096 (14)
H36	0.7530	-0.2390	1.0995	0.132*
C37	0.6703 (7)	-0.2950 (11)	1.0249 (7)	0.1096 (14)
H37	0.6403	-0.2876	1.0517	0.132*
C38	0.6407 (7)	-0.3338 (12)	0.9634 (7)	0.1096 (14)
H38	0.5934	-0.3584	0.9491	0.132*
C39	0.6811 (6)	-0.3370 (12)	0.9211 (7)	0.1096 (14)
H39	0.6609	-0.3544	0.8762	0.132*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
La1	0.0460 (2)	0.0376 (2)	0.0358 (2)	-0.00143 (13)	0.00419 (15)	0.00054 (13)
O1	0.064 (3)	0.057 (3)	0.052 (2)	0.005 (2)	0.019 (2)	0.003 (2)
O2	0.068 (3)	0.066 (3)	0.050 (3)	0.008 (2)	0.019 (2)	0.014 (2)
O4	0.074 (3)	0.047 (3)	0.047 (2)	-0.003 (2)	0.014 (2)	-0.008 (2)
O5	0.091 (4)	0.067 (3)	0.045 (3)	-0.029 (3)	0.021 (2)	0.000 (2)
O7	0.049 (2)	0.047 (3)	0.057 (3)	-0.003 (2)	0.0016 (19)	-0.003 (2)
O8	0.056 (3)	0.061 (3)	0.053 (3)	-0.003 (2)	0.002 (2)	0.007 (2)
N1	0.054 (3)	0.056 (3)	0.058 (3)	0.005 (3)	0.006 (3)	-0.005 (3)
N2	0.066 (4)	0.054 (4)	0.042 (3)	0.004 (3)	0.003 (3)	0.002 (2)
C1	0.064 (5)	0.094 (7)	0.062 (5)	0.009 (4)	0.017 (4)	-0.002 (4)
C2	0.057 (5)	0.147 (10)	0.087 (7)	-0.003 (5)	0.025 (5)	-0.016 (6)
C3	0.054 (5)	0.123 (10)	0.129 (10)	-0.005 (5)	0.023 (6)	-0.013 (7)
C4	0.057 (5)	0.105 (7)	0.088 (7)	0.007 (5)	-0.005 (4)	-0.022 (6)
C5	0.062 (4)	0.042 (4)	0.073 (5)	0.007 (3)	0.007 (3)	-0.007 (3)
C6	0.055 (6)	0.207 (17)	0.137 (12)	-0.001 (7)	0.004 (6)	-0.023 (10)
C7	0.074 (6)	0.153 (10)	0.079 (6)	0.043 (6)	-0.022 (5)	0.007 (6)
C8	0.082 (6)	0.081 (5)	0.062 (5)	0.020 (5)	-0.018 (4)	-0.010 (4)
C9	0.067 (4)	0.049 (4)	0.050 (4)	0.001 (3)	-0.009 (3)	-0.007 (3)
C10	0.119 (8)	0.091 (7)	0.055 (5)	0.016 (6)	-0.015 (5)	-0.002 (4)
C11	0.130 (8)	0.090 (7)	0.043 (4)	0.001 (6)	0.003 (5)	0.014 (4)
C12	0.091 (6)	0.060 (5)	0.055 (4)	-0.003 (4)	0.006 (4)	0.009 (3)
C13	0.054 (4)	0.045 (4)	0.050 (4)	-0.005 (3)	0.012 (3)	0.001 (3)
C14	0.061 (2)	0.063 (3)	0.053 (2)	0.0072 (19)	0.0242 (18)	0.0129 (18)
C15	0.061 (2)	0.063 (3)	0.053 (2)	0.0072 (19)	0.0242 (18)	0.0129 (18)
C16	0.061 (2)	0.063 (3)	0.053 (2)	0.0072 (19)	0.0242 (18)	0.0129 (18)
C17	0.093 (6)	0.121 (8)	0.083 (6)	0.008 (6)	0.047 (5)	-0.001 (5)
C18	0.093 (7)	0.125 (10)	0.121 (8)	-0.009 (6)	0.057 (6)	-0.007 (7)

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C19	0.151 (10)	0.096 (8)	0.151 (10)	-0.015 (7)	0.111 (9)	-0.004 (7)
C20	0.165 (11)	0.123 (9)	0.107 (8)	0.021 (9)	0.087 (9)	0.038 (7)
C21	0.113 (7)	0.099 (7)	0.098 (7)	0.000 (6)	0.066 (6)	0.017 (6)
C22	0.064 (4)	0.039 (4)	0.053 (4)	-0.002 (3)	0.016 (3)	0.001 (3)
C23	0.074 (2)	0.052 (2)	0.0390 (18)	-0.0157 (18)	0.0188 (17)	-0.0037 (15)
C24	0.074 (2)	0.052 (2)	0.0390 (18)	-0.0157 (18)	0.0188 (17)	-0.0037 (15)
C25	0.074 (2)	0.052 (2)	0.0390 (18)	-0.0157 (18)	0.0188 (17)	-0.0037 (15)
C26	0.084 (5)	0.110 (7)	0.063 (5)	-0.039 (5)	0.026 (4)	-0.013 (5)
C27	0.157 (11)	0.167 (11)	0.066 (6)	-0.065 (9)	0.052 (7)	-0.010 (7)
C28	0.132 (9)	0.155 (11)	0.069 (6)	-0.014 (8)	0.049 (6)	0.016 (7)
C29	0.130 (8)	0.117 (8)	0.053 (5)	-0.017 (7)	0.018 (5)	-0.002 (5)
C30	0.092 (6)	0.092 (6)	0.060 (5)	-0.030 (5)	0.016 (4)	-0.014 (4)
C31	0.050 (3)	0.062 (4)	0.039 (3)	0.002 (3)	0.005 (3)	-0.001 (3)
C32	0.060 (4)	0.061 (5)	0.060 (4)	0.011 (3)	0.007 (3)	-0.006 (3)
C33	0.108 (3)	0.091 (3)	0.135 (4)	0.000 (2)	0.044 (3)	0.017 (3)
C34	0.108 (3)	0.091 (3)	0.135 (4)	0.000 (2)	0.044 (3)	0.017 (3)
C35	0.108 (3)	0.091 (3)	0.135 (4)	0.000 (2)	0.044 (3)	0.017 (3)
C36	0.108 (3)	0.091 (3)	0.135 (4)	0.000 (2)	0.044 (3)	0.017 (3)
C37	0.108 (3)	0.091 (3)	0.135 (4)	0.000 (2)	0.044 (3)	0.017 (3)
C38	0.108 (3)	0.091 (3)	0.135 (4)	0.000 (2)	0.044 (3)	0.017 (3)
C39	0.108 (3)	0.091 (3)	0.135 (4)	0.000 (2)	0.044 (3)	0.017 (3)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

La1—O1	2.504 (4)	C15—H15B	0.9700
La1—O4	2.478 (4)	C16—C17	1.341 (11)
La1—O7	2.615 (4)	C16—C21	1.401 (11)
La1—O8	2.908 (6)	C17—C18	1.419 (13)
La1—N1	2.717 (6)	C17—H17	0.9300
La1—N2	2.749 (5)	C18—C19	1.396 (16)
La1—O8 <sup>i</sup>	2.440 (5)	C18—H18	0.9300
La1—O2 <sup>i</sup>	2.566 (4)	C19—C20	1.317 (15)
La1—O5 <sup>ii</sup>	2.570 (4)	C19—H19	0.9300
O1—C13	1.237 (7)	C20—C21	1.429 (12)
O2—C13	1.276 (7)	C20—H20	0.9300
O2—La1 <sup>i</sup>	2.566 (4)	C21—H21	0.9300
O4—C22	1.275 (8)	C22—C23	1.524 (8)
O5—C22	1.250 (8)	C23—C24	1.448 (8)
O5—La1 <sup>ii</sup>	2.570 (4)	C23—H23B	0.9700
O7—C31	1.263 (8)	C23—H23A	0.9700
O8—C31	1.295 (8)	C24—C25	1.366 (8)
O8—La1 <sup>i</sup>	2.440 (5)	C24—H24A	0.9700
N1—C1	1.344 (10)	C24—H24B	0.9700
N1—C5	1.367 (9)	C25—C26	1.374 (10)
N2—C9	1.345 (10)	C25—C30	1.425 (9)
N2—C12	1.346 (9)	C26—C27	1.397 (12)
C1—C2	1.365 (11)	C26—H26	0.9300
C1—H1	0.9300	C27—C28	1.391 (15)

C2—C3	1.402 (15)	C27—H27	0.9300
C2—H2	0.9300	C28—C29	1.381 (14)
C3—C4	1.390 (14)	C28—H28	0.9300
C3—H3	0.9300	C29—C30	1.397 (11)
C4—C5	1.404 (11)	C29—H29	0.9300
C4—C6	1.483 (15)	C30—H30	0.9300
C5—C9	1.453 (11)	C31—C32	1.521 (10)
C6—C7	1.458 (16)	C32—C33	1.376 (13)
C6—H6	0.9300	C32—H32A	0.9700
C7—C8	1.385 (14)	C32—H32B	0.9700
C7—H7	0.9300	C33—C34	1.319 (16)
C8—C10	1.412 (13)	C33—H33A	0.9700
C8—C9	1.444 (10)	C33—H33B	0.9700
C10—C11	1.332 (12)	C34—C39	1.390 (16)
C10—H10	0.9300	C34—C35	1.430 (18)
C11—C12	1.407 (11)	C35—C36	1.467 (15)
C11—H11	0.9300	C35—H35	0.9300
C12—H12	0.9300	C36—C37	1.335 (15)
C13—C14	1.527 (8)	C36—H36	0.9300
C14—C15	1.400 (8)	C37—C38	1.309 (16)
C14—H14A	0.9700	C37—H37	0.9300
C14—H14B	0.9700	C38—C39	1.354 (15)
C15—C16	1.370 (8)	C38—H38	0.9300
C15—H15A	0.9700	C39—H39	0.9300
O1—La1—O4	146.17 (15)	C13—C14—H14B	109.7
O1—La1—O7	71.74 (14)	H14A—C14—H14B	108.2
O1—La1—O8	64.45 (14)	C16—C15—C14	116.7 (6)
O4—La1—O7	140.47 (15)	C16—C15—H15A	108.1
O4—La1—O8	140.10 (13)	C14—C15—H15A	108.1
O7—La1—O8	47.01 (13)	C16—C15—H15B	108.1
O1—La1—N1	126.56 (16)	C14—C15—H15B	108.1
O4—La1—N1	77.48 (16)	H15A—C15—H15B	107.3
O7—La1—N1	64.84 (16)	C17—C16—C15	113.1 (7)
O8—La1—N1	102.67 (16)	C17—C16—C21	122.8 (7)
O1—La1—N2	80.59 (16)	C15—C16—C21	124.1 (7)
O4—La1—N2	96.40 (15)	C16—C17—C18	118.1 (10)
O7—La1—N2	75.47 (15)	C16—C17—H17	121.0
O8—La1—N2	118.56 (14)	C18—C17—H17	121.0
N1—La1—N2	59.97 (18)	C19—C18—C17	119.4 (10)
O8 <sup>i</sup> —La1—O4	87.64 (17)	C19—C18—H18	120.3
O8 <sup>i</sup> —La1—O1	79.22 (15)	C17—C18—H18	120.3
O8 <sup>i</sup> —La1—O2 <sup>i</sup>	72.78 (15)	C20—C19—C18	122.0 (10)
O4—La1—O2 <sup>i</sup>	76.59 (15)	C20—C19—H19	119.0
O1—La1—O2 <sup>i</sup>	127.14 (16)	C18—C19—H19	119.0
O8 <sup>i</sup> —La1—O5 <sup>ii</sup>	80.04 (17)	C19—C20—C21	119.9 (11)
O4—La1—O5 <sup>ii</sup>	75.77 (15)	C19—C20—H20	120.1
O1—La1—O5 <sup>ii</sup>	71.35 (15)	C21—C20—H20	120.1

## supplementary materials

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O2 <sup>i</sup> —La1—O5 <sup>ii</sup>	141.66 (15)	C16—C21—C20	117.6 (9)
O8 <sup>i</sup> —La1—O7	119.25 (17)	C16—C21—H21	121.2
O2 <sup>i</sup> —La1—O7	84.17 (15)	C20—C21—H21	121.2
O5 <sup>ii</sup> —La1—O7	133.41 (14)	O5—C22—O4	128.5 (6)
O8 <sup>i</sup> —La1—N1	149.81 (16)	O5—C22—C23	118.2 (6)
O2 <sup>i</sup> —La1—N1	78.24 (16)	O4—C22—C23	113.2 (5)
O5 <sup>ii</sup> —La1—N1	120.31 (18)	C24—C23—C22	112.2 (5)
O8 <sup>i</sup> —La1—N2	149.02 (17)	C24—C23—H23B	109.2
O2 <sup>i</sup> —La1—N2	138.05 (17)	C22—C23—H23B	109.2
O5 <sup>ii</sup> —La1—N2	71.35 (17)	C24—C23—H23A	109.2
O8 <sup>i</sup> —La1—O8	72.45 (18)	C22—C23—H23A	109.2
O2 <sup>i</sup> —La1—O8	64.71 (14)	H23B—C23—H23A	107.9
O5 <sup>ii</sup> —La1—O8	131.14 (15)	C25—C24—C23	118.9 (6)
C13—O1—La1	129.9 (4)	C25—C24—H24A	107.6
C13—O2—La1 <sup>i</sup>	138.8 (4)	C23—C24—H24A	107.6
C22—O4—La1	151.8 (4)	C25—C24—H24B	107.6
C22—O5—La1 <sup>ii</sup>	148.9 (4)	C23—C24—H24B	107.6
C31—O7—La1	103.6 (4)	H24A—C24—H24B	107.0
C31—O8—La1 <sup>i</sup>	161.9 (5)	C24—C25—C26	123.2 (6)
C31—O8—La1	88.9 (4)	C24—C25—C30	115.9 (6)
La1 <sup>i</sup> —O8—La1	107.55 (18)	C26—C25—C30	121.0 (6)
C1—N1—C5	119.5 (6)	C25—C26—C27	118.4 (8)
C1—N1—La1	118.8 (5)	C25—C26—H26	120.8
C5—N1—La1	120.1 (5)	C27—C26—H26	120.8
C9—N2—C12	115.9 (6)	C28—C27—C26	121.2 (10)
C9—N2—La1	122.0 (4)	C28—C27—H27	119.4
C12—N2—La1	121.7 (5)	C26—C27—H27	119.4
N1—C1—C2	121.9 (8)	C29—C28—C27	120.6 (9)
N1—C1—H1	119.0	C29—C28—H28	119.7
C2—C1—H1	119.0	C27—C28—H28	119.7
C1—C2—C3	118.3 (9)	C28—C29—C30	119.2 (9)
C1—C2—H2	120.9	C28—C29—H29	120.4
C3—C2—H2	120.9	C30—C29—H29	120.4
C4—C3—C2	122.2 (9)	C29—C30—C25	119.4 (8)
C4—C3—H3	118.9	C29—C30—H30	120.3
C2—C3—H3	118.9	C25—C30—H30	120.3
C3—C4—C5	115.3 (8)	O7—C31—O8	120.3 (6)
C3—C4—C6	121.5 (9)	O7—C31—C32	122.1 (6)
C5—C4—C6	123.2 (10)	O8—C31—C32	117.6 (6)
N1—C5—C4	122.9 (8)	C33—C32—C31	115.8 (7)
N1—C5—C9	119.9 (6)	C33—C32—H32A	108.3
C4—C5—C9	117.2 (7)	C31—C32—H32A	108.3
C7—C6—C4	117.3 (9)	C33—C32—H32B	108.3
C7—C6—H6	121.3	C31—C32—H32B	108.3
C4—C6—H6	121.3	H32A—C32—H32B	107.4

C8—C7—C6	119.4 (8)	C34—C33—C32	117.2 (12)
C8—C7—H7	120.3	C34—C33—H33A	108.0
C6—C7—H7	120.3	C32—C33—H33A	108.0
C7—C8—C10	121.0 (9)	C34—C33—H33B	108.0
C7—C8—C9	122.7 (9)	C32—C33—H33B	108.0
C10—C8—C9	116.3 (8)	H33A—C33—H33B	107.2
N2—C9—C8	123.7 (8)	C33—C34—C39	113.2 (14)
N2—C9—C5	116.3 (6)	C33—C34—C35	125.2 (13)
C8—C9—C5	120.1 (8)	C39—C34—C35	121.6 (12)
C11—C10—C8	120.2 (8)	C34—C35—C36	115.5 (12)
C11—C10—H10	119.9	C34—C35—H35	122.2
C8—C10—H10	119.9	C36—C35—H35	122.2
C10—C11—C12	119.4 (9)	C37—C36—C35	115.6 (13)
C10—C11—H11	120.3	C37—C36—H36	122.2
C12—C11—H11	120.3	C35—C36—H36	122.2
N2—C12—C11	124.2 (9)	C38—C37—C36	129.3 (13)
N2—C12—H12	117.9	C38—C37—H37	115.3
C11—C12—H12	117.9	C36—C37—H37	115.3
O1—C13—O2	128.8 (6)	C37—C38—C39	117.9 (13)
O1—C13—C14	110.8 (5)	C37—C38—H38	121.1
O2—C13—C14	120.3 (6)	C39—C38—H38	121.1
C15—C14—C13	109.6 (5)	C38—C39—C34	119.8 (14)
C15—C14—H14A	109.7	C38—C39—H39	120.1
C13—C14—H14A	109.7	C34—C39—H39	120.1
C15—C14—H14B	109.7		

Symmetry codes: (i)  $-x+2, -y, -z+2$ ; (ii)  $-x+2, -y+1, -z+2$ .

*Hydrogen-bond geometry* ( $\text{\AA}, ^\circ$ )

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C1—H1...O2 <sup>i</sup>	0.93	2.44	3.138 (10)	132
C12—H12...O5 <sup>ii</sup>	0.93	2.53	3.087 (9)	119
C32—H32B...O4 <sup>iii</sup>	0.97	2.48	3.435 (9)	167
C10—H10...O7 <sup>iv</sup>	0.93	2.39	3.279 (9)	159

Symmetry codes: (i)  $-x+2, -y, -z+2$ ; (ii)  $-x+2, -y+1, -z+2$ ; (iii)  $x, y-1, z$ ; (iv)  $-x+3/2, y+1/2, -z+3/2$ .

Fig. 1

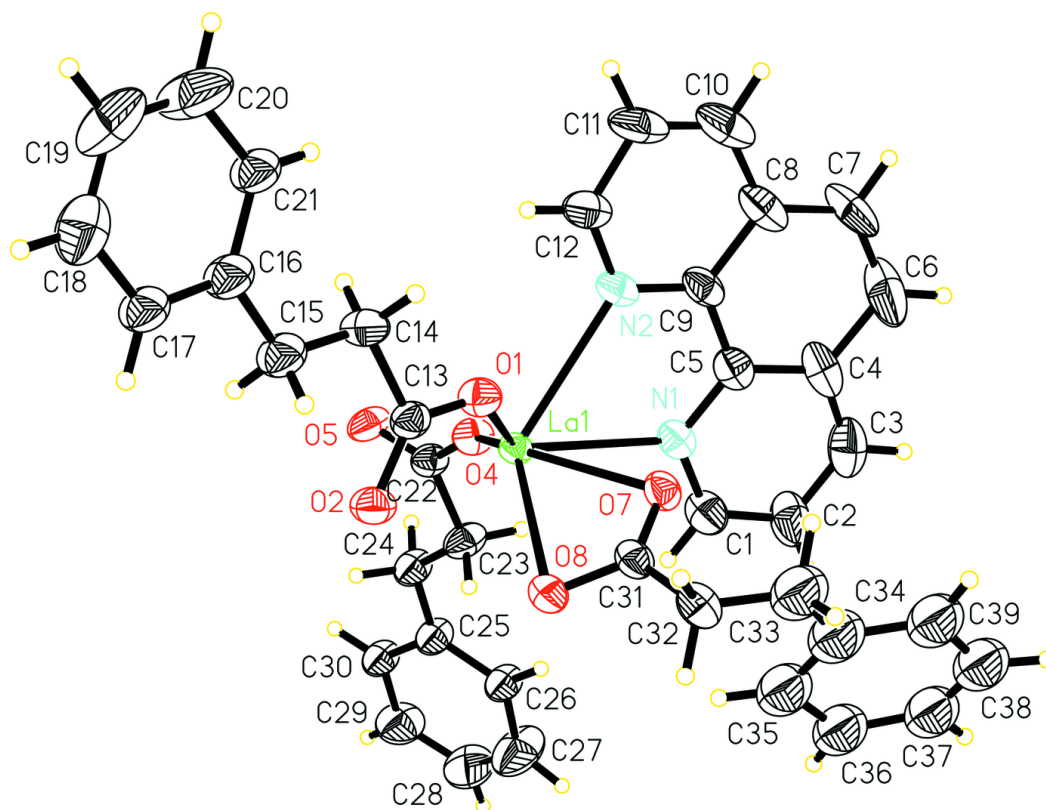


Fig. 2

